

http://www.ncbi.nlm.nih.gov/peptidome/

Entrez

Entrez search results for "peptidome". The results page shows a list of studies and samples. A red arrow points from the top of the page down towards the "Samples" section.

Abstract

Building on extensive experience in creating biological scientific data repositories to provide an integrated approach to the use of gene and protein sequence information, the National Center for Biotechnology Information (NCBI) has created a new project to collect and distribute mass spectrometry peptide and protein identification data. The results are organized into Studies and Samples. A Sample describes all results common to a given biological sample, while a Study organizes Samples into the meaningful datasets which make up an experiment. In addition to data storage, web-based interfaces are available to help users query, browse and download individual peptides, proteins, samples or entire studies. The goal is to make data submission as simple as possible, while encouraging a high level of experimental annotation. The burden of data submission is minimized by accepting common file formats from which required information is extracted. Data submission involves filling out a spreadsheet with basic descriptive information and packaging it along with original peak list files and output files from the search engine analysis programs. Results and conclusion-level information are captured, together with raw data and descriptive information to enable understanding of the experiment and analysis of the underlying data. Results are integrated with other NCBI data using the Entrez cross-database search system, allowing dissemination of information beyond the MS Proteomics community. In addition, NCBI and the European Bioinformatics Institute, together with the other Protein Exchange members, are also working on data sharing and distribution.

Genome Browser

Genome Browser interface showing a genomic track for a protein. A red arrow points from the top of the page down towards the "Samples" section.

Spectral data is not stored in the database, rather it is converted from mzXML to mzPFS. This allows all or the MS data for an entire sample to be stored in a single file which is smaller than a BZIP2 compressed XML file, and yet still allow fast retrieval of an individual spectrum.

Peptide identifications may come from one or more methods, including de novo or some other currently unknown method. The criteria for selecting valid identifications is left to the submitter. This is done by requiring a finalized list, and not the criteria itself, such as cutoff scores.

Samples

Samples interface showing a list of samples. A red arrow points from the top of the page down towards the "Studies" section.

The genome browser allows results to be viewed graphically, and experimental data to be compared and contrasted with other annotations.

Identifying proteins from mass spectral data can be thought of as two separate problems:

1. Identify peptides from spectra.
2. Identify proteins from peptides.

The resource is set up to reflect this dichotomy and accurately record the original solution from each submitter.

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